dabl

Automatic ML with a human in the loop

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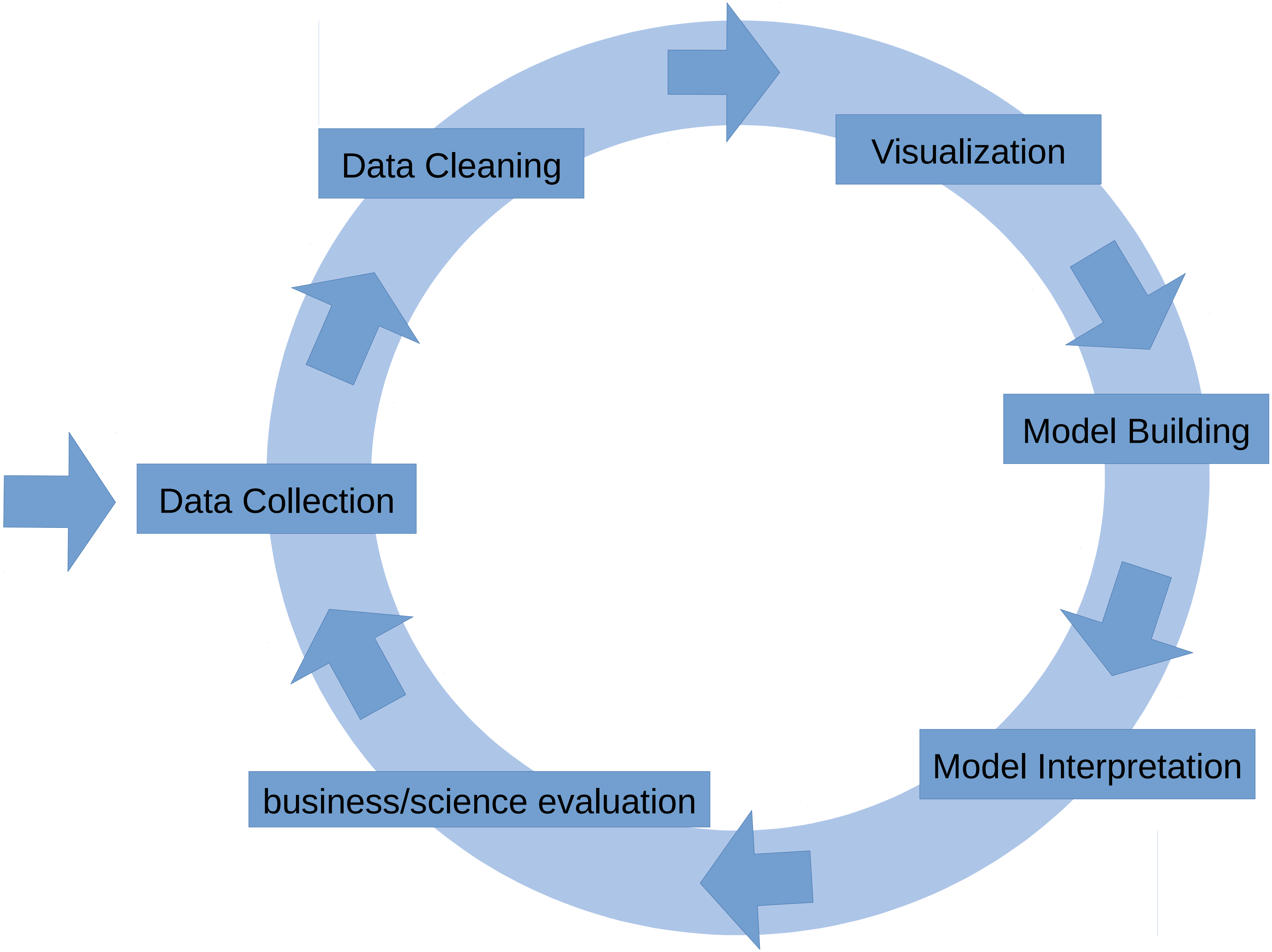
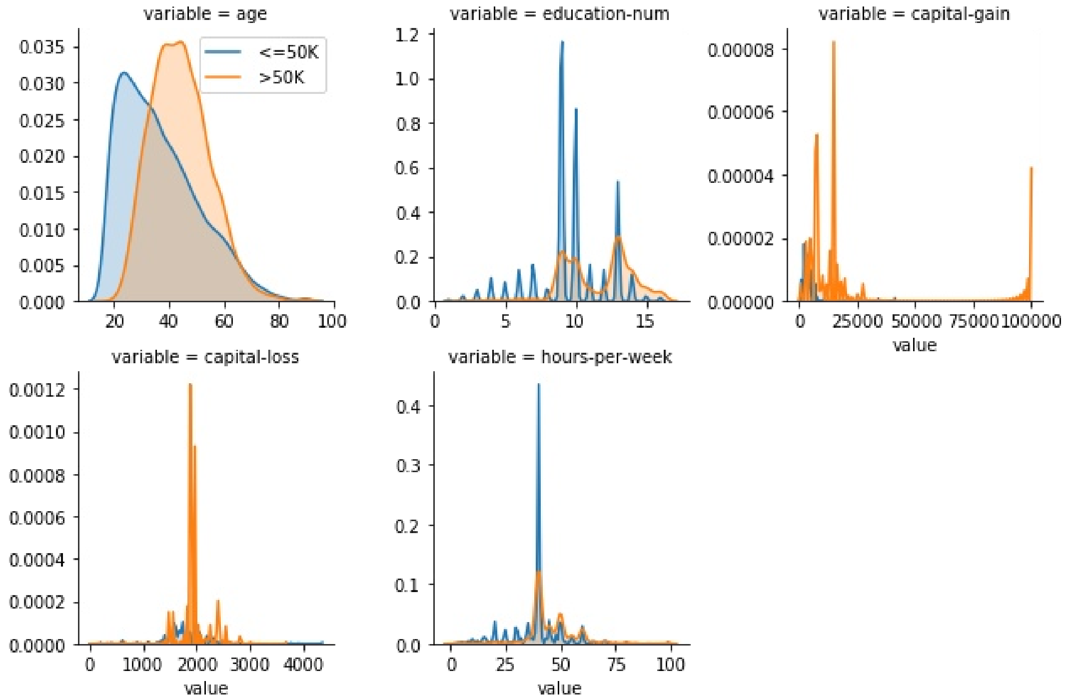
A real world ML workflow



ML with sklearn & pandas

```
import pandas as pd
import seaborn as sns

data = pd.read_csv("adult.csv", index_col=0)

cols = data.columns[data.dtypes != object].tolist() + ['income']
df = data.loc[:, cols].melt("income")
g = sns.FacetGrid(df, col='variable', hue='income',
                  sharey=False, sharex=False, col_wrap=3)
g = g.map(sns.kdeplot, "value", shade=True)
g.axes[0].legend()
```



ML with sklearn & pandas

```
from sklearn.compose import ColumnTransformer
from sklearn.preprocessing import StandardScaler, OneHotEncoder
from sklearn.pipeline import Pipeline
from sklearn.impute import SimpleImputer
from sklearn.model_selection import GridSearchCV
from sklearn.linear_model import LogisticRegression

categorical_columns = data_features.dtypes == object

cont_pipe = Pipeline([('scaler', StandardScaler()),
                      ('imputer', SimpleImputer(strategy='median', add_indicator=True))])
cat_pipe = Pipeline([('ohe', OneHotEncoder(handle_unknown='ignore')),
                     ('imputer', SimpleImputer(strategy='most_frequent', add_indicator=True))])

pre = ColumnTransformer([('categorical', cat_pipe, categorical_columns),
                         ('continuous', cont_pipe, ~categorical_columns),
                        ])

model = Pipeline([('preprocessing', pre), ('clf', LogisticRegression())])
param_grid = {'clf__C': np.logspace(-3, 3, 7)}
grid_search = GridSearchCV(model, param_grid=param_grid)
grid_search.fit(X_train, y_train)
```

Current Automatic ML frameworks

Example

```
>>> import autosklearn.classification
>>> import sklearn.model_selection
>>> import sklearn.datasets
>>> import sklearn.metrics
>>> X, y = sklearn.datasets.load_digits(return_X_y=True)
>>> X_train, X_test, y_train, y_test = \
        sklearn.model_selection.train_test_split(X, y, random_state=1)
>>> automl = autosklearn.classification.AutoSklearnClassifier()
>>> automl.fit(X_train, y_train)
>>> y_hat = automl.predict(X_test)
>>> print("Accuracy score", sklearn.metrics.accuracy_score(y_test, y_hat))
```

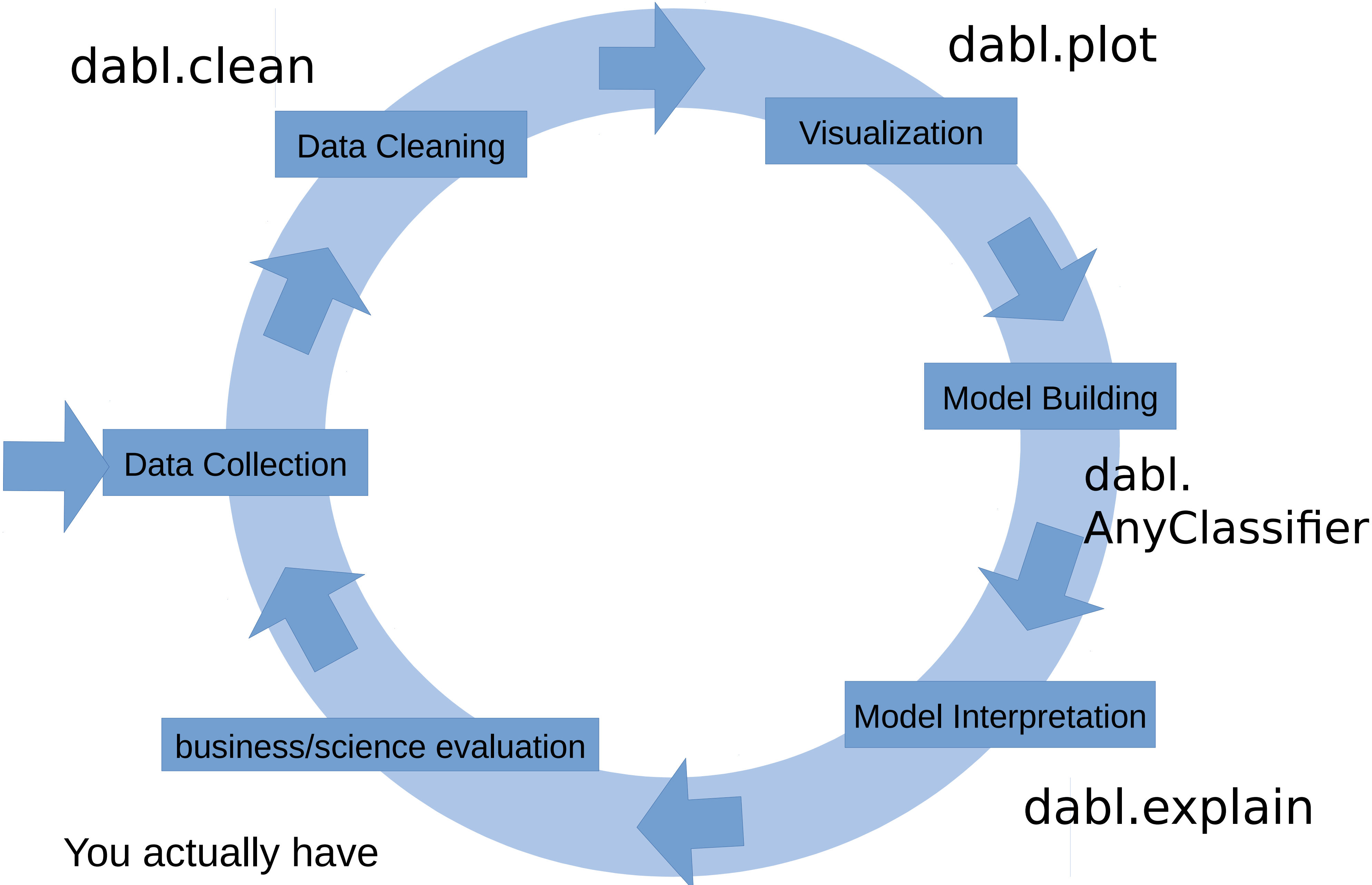
This will run for one hour and should result in an accuracy above 0.98.

[redacted]

A NEW HOPE

data
analysis
baseline
library

A NEW HOPE



You actually have
to think, sorry.

Data cleaning
& preprocessing

```python
import dabl
ames_df = dabl.datasets.load_ames()
ames_df.head()
```

	Order	PID	MS SubClass	MS Zoning	Lot Frontage	Lot Area	Street	Alley	Lot Shape	Land Contour	...	Pool Area	Pool QC	Fence	Misc Feature	Misc Val	Mo Sold	Yr Sold	Sale Type	Sale Condition
0	1	526301100	20	RL	141.0	31770	Pave	NaN	IR1	Lvl	...	0	NaN	NaN	NaN	0	5	2010	WD	Normal
1	2	526350040	20	RH	80.0	11622	Pave	NaN	Reg	Lvl	...	0	NaN	MnPrv	NaN	0	6	2010	WD	Normal
2	3	526351010	20	RL	81.0	14267	Pave	NaN	IR1	Lvl	...	0	NaN	NaN	Gar2	12500	6	2010	WD	Normal
3	4	526353030	20	RL	93.0	11160	Pave	NaN	Reg	Lvl	...	0	NaN	NaN	NaN	0	4	2010	WD	Normal
4	5	527105010	60	RL	74.0	13830	Pave	NaN	IR1	Lvl	...	0	NaN	MnPrv	NaN	0	3	2010	WD	Normal

5 rows × 82 columns

```python
clean_df = dabl.clean(ames_df, verbose=2)
```

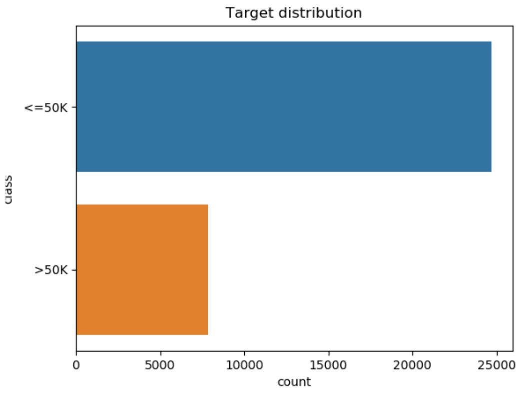
```
Detected feature types:
11 float, 28 int, 43 object, 0 date, 0 other
Interpreted as:
continuous      23
dirty_float      0
low_card_int     6
categorical     40
date             0
free_string      0
useless         13
dtype: int64
WARN dropped useless columns: ['Order', 'Street', 'Utilities', 'Land Slope', 'Condition 2', 'Roof Matl', 'Heating', 'Low Qual
Fin SF', 'Kitchen AbvGr', 'Garage Cond', '3Ssn Porch', 'Pool Area', 'Misc Val']
```

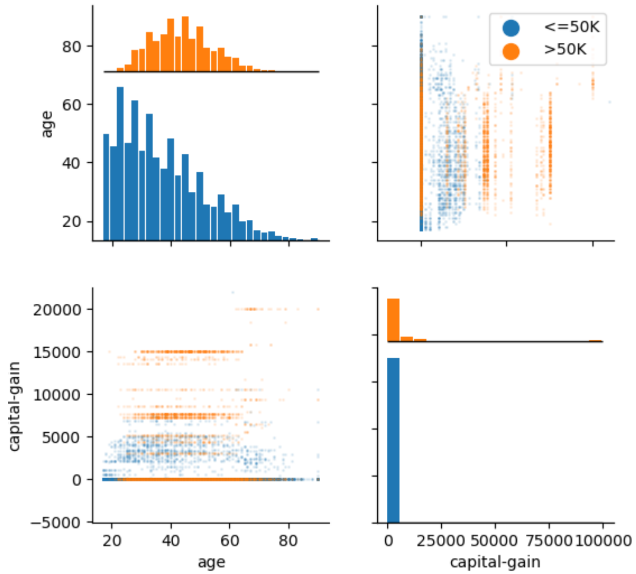
dabl.clean

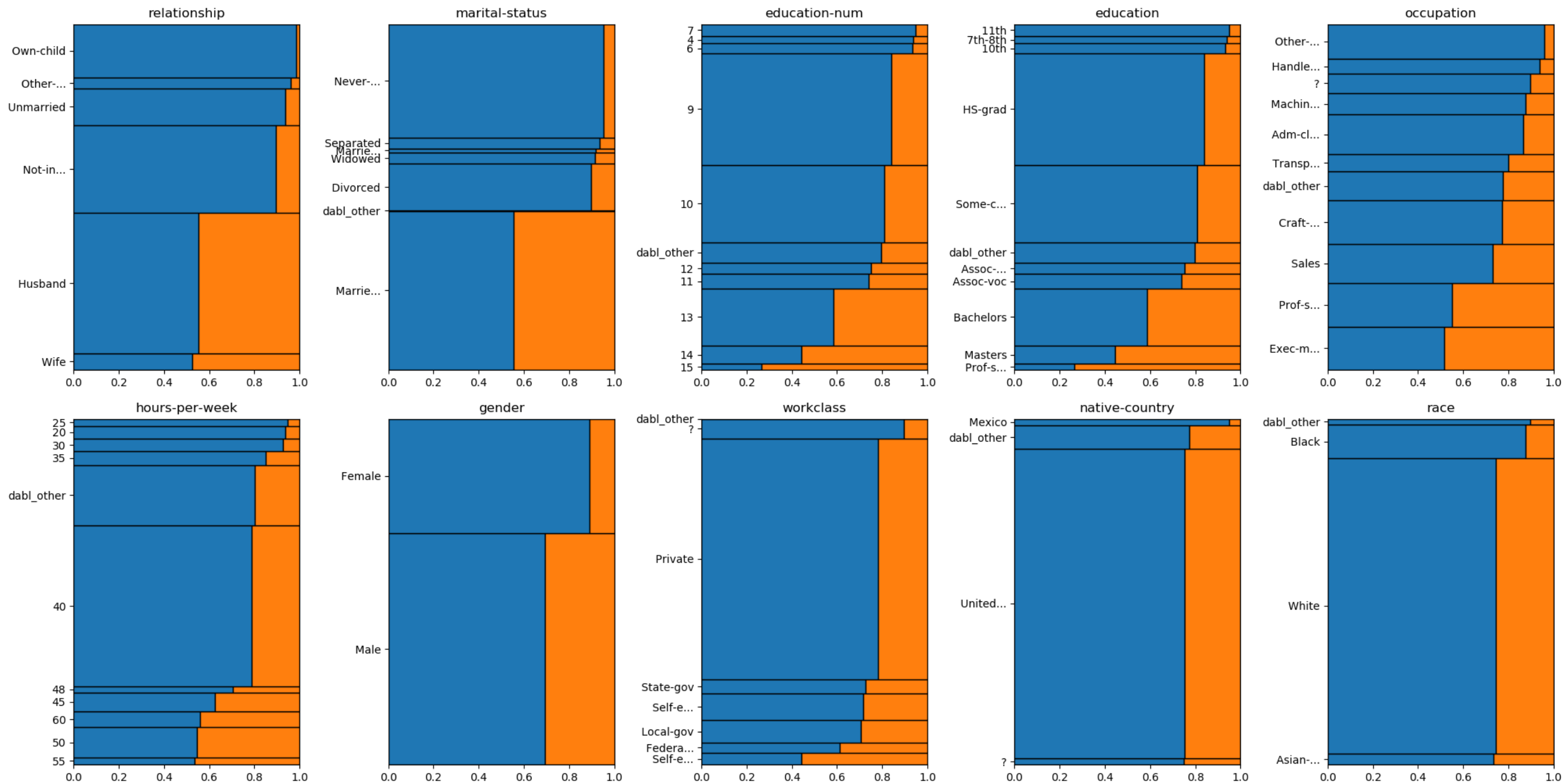
- Detect types (can overwrite)
- Detect Missing / rare values
- Detect ordinal vs categorical
- Detect near-constant
- Detect index

Visualization

```
data = pd.read_csv("adult.csv", index_col=0)
plot(data, 'income', scatter_alpha=.1)
```

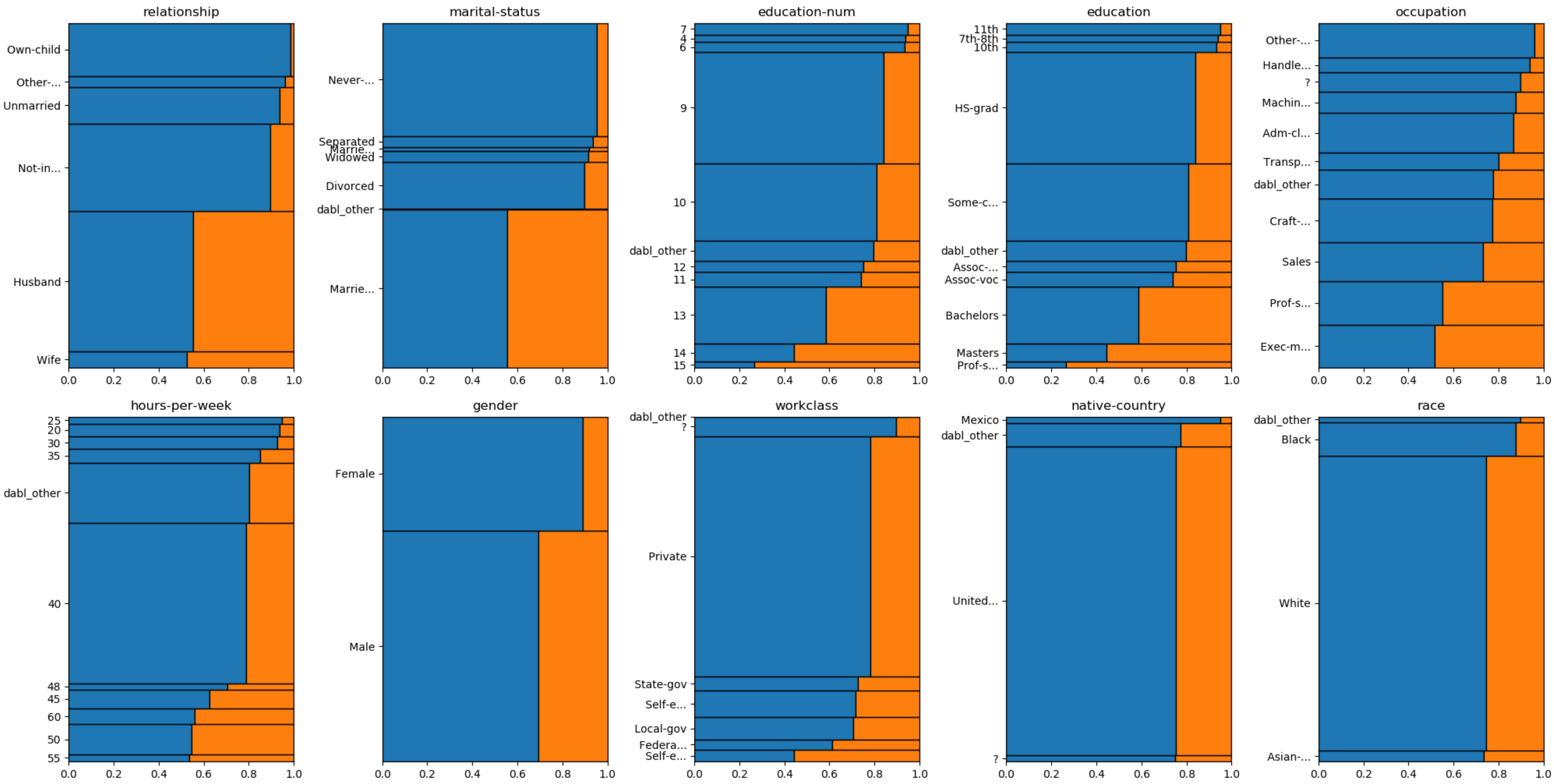




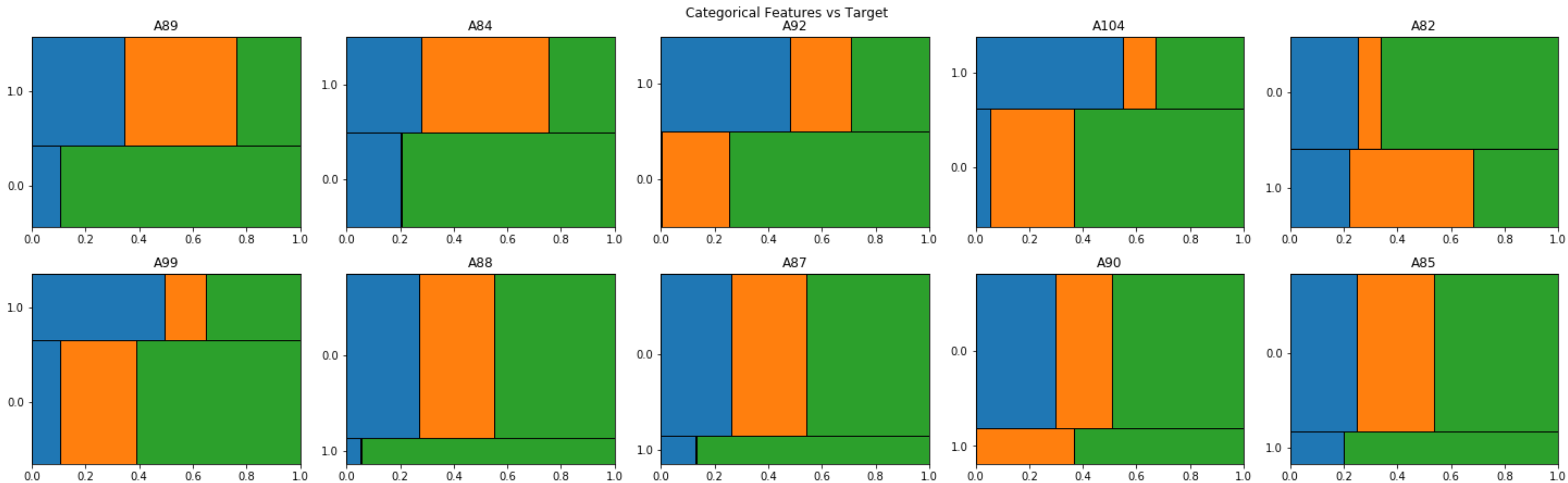


Univariate plots

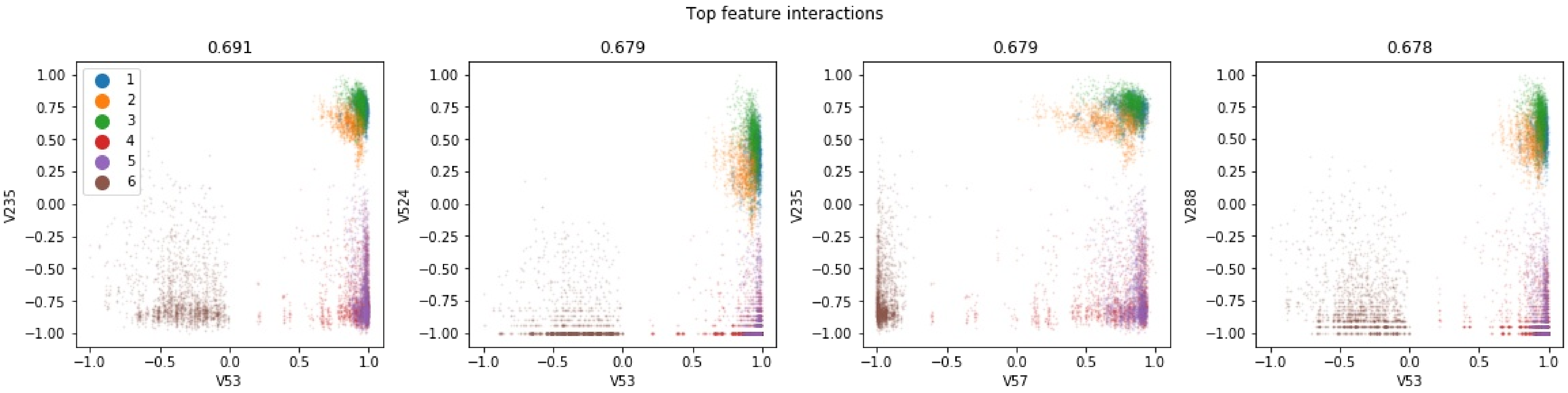
Mosaic Plots



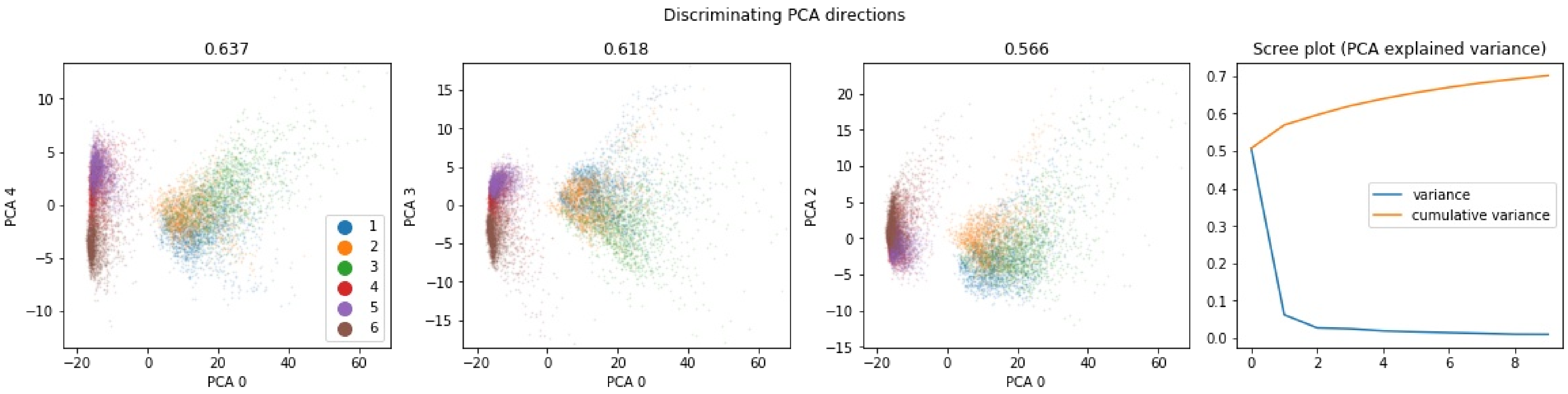
Mosaic Plots



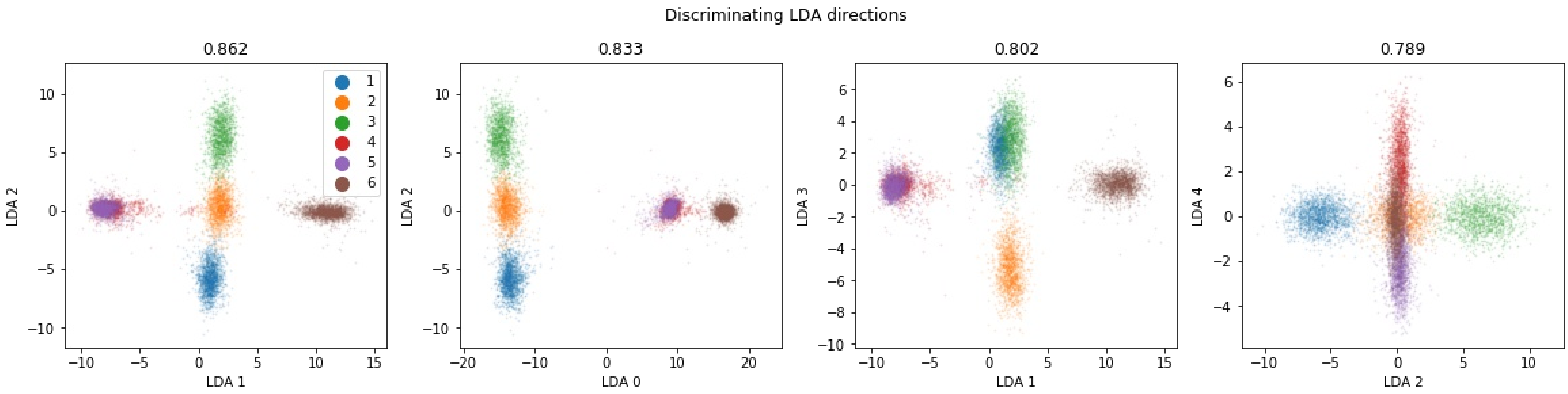
Pairwise Plots



Principal Component Analysis



Linear Discriminant Analysis



Preprocessing

```
X, y = ames_df.drop('SalePrice', axis=1), ames_df.SalePrice
ep =  EasyPreprocessor().fit(X, y)
```

```
/home/andy/checkout/dabl/dabl/preprocessing.py:258: UserWarning: Discarding near-constan
'Land Slope', 'Condition 2', 'Roof Matl', 'Heating', 'Low Qual Fin SF', 'Kitchen AbvGr',
rea', 'Misc Val']
  near_constant.index[near_constant].tolist()))
```

```
ep.ct_
```

```
ColumnTransformer(n_jobs=None, remainder='drop', sparse_threshold=0.1,
                  transformer_weights=None,
                  transformers=[('continuous',
                                 Pipeline(memory=None,
                                          steps=[('simpleimputer',
                                                  SimpleImputer(add_indicator=False,
                                                                copy=True,
                                                                fill_value=None,
                                                                missing_values=nan,
                                                                strategy='median',
                                                                verbose=0)),
                                                 ('standardscaler',
                                                  StandardScaler(copy=True,
                                                                 with_mean=True,
                                                                 with_std=True))],...
```

Simple Prototypes

- Dummy Models
- Naive Bayes
- Stumps
- Linear Models

```python
from dabl import SimpleClassifier
data = pd.read_csv("adult.csv", index_col=0)
SimpleClassifier().fit(data, target_col='income')
```

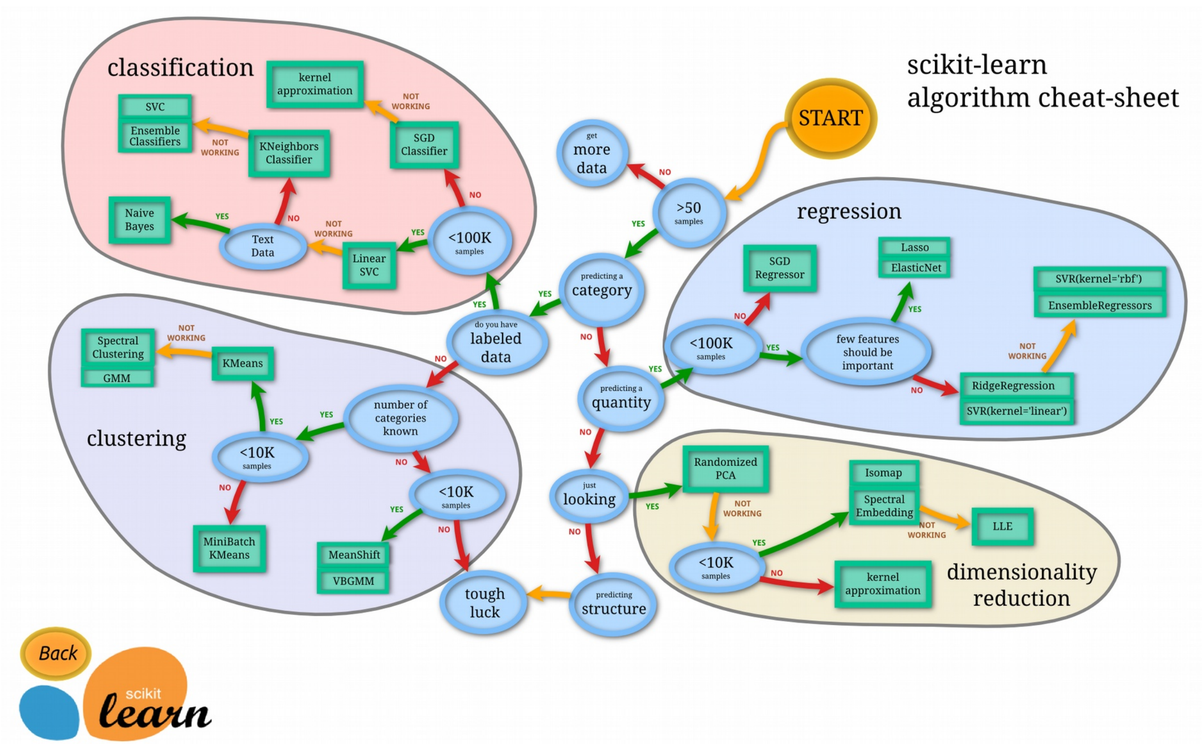
Either X, y
Or dataframe, target_col

```
/home/andy/checkout/dabl/dabl/preprocessing.py:258: UserWarning: Discarding near-constant featur
  near_constant.index[near_constant].tolist()))
Running DummyClassifier(strategy='prior')
accuracy: 0.759 average_precision: 0.241 f1_macro: 0.432 recall_macro: 0.500 roc_auc: 0.500
=== new best DummyClassifier(strategy='prior') (using recall_macro):
accuracy: 0.759 average_precision: 0.241 f1_macro: 0.432 recall_macro: 0.500 roc_auc: 0.500

Running GaussianNB()
accuracy: 0.407 average_precision: 0.288 f1_macro: 0.405 recall_macro: 0.605 roc_auc: 0.607
=== new best GaussianNB() (using recall_macro):
accuracy: 0.407 average_precision: 0.288 f1_macro: 0.405 recall_macro: 0.605 roc_auc: 0.607

Running MultinomialNB()
accuracy: 0.831 average_precision: 0.773 f1_macro: 0.787 recall_macro: 0.815 roc_auc: 0.908
=== new best MultinomialNB() (using recall_macro):
accuracy: 0.831 average_precision: 0.773 f1_macro: 0.787 recall_macro: 0.815 roc_auc: 0.908

Running DecisionTreeClassifier(class_weight='balanced', max_depth=1)
accuracy: 0.710 average_precision: 0.417 f1_macro: 0.682 recall_macro: 0.759 roc_auc: 0.759
Running DecisionTreeClassifier(class_weight='balanced', max_depth=5)
accuracy: 0.784 average_precision: 0.711 f1_macro: 0.750 recall_macro: 0.811 roc_auc: 0.894
Running DecisionTreeClassifier(class_weight='balanced', min_impurity_decrease=0.01)
accuracy: 0.718 average_precision: 0.561 f1_macro: 0.693 recall_macro: 0.779 roc_auc: 0.848
Running LogisticRegression(C=0.1, class_weight='balanced')
accuracy: 0.819 average_precision: 0.789 f1_macro: 0.783 recall_macro: 0.832 roc_auc: 0.915
=== new best LogisticRegression(C=0.1, class_weight='balanced') (using recall_macro):
accuracy: 0.819 average_precision: 0.789 f1_macro: 0.783 recall_macro: 0.832 roc_auc: 0.915
```

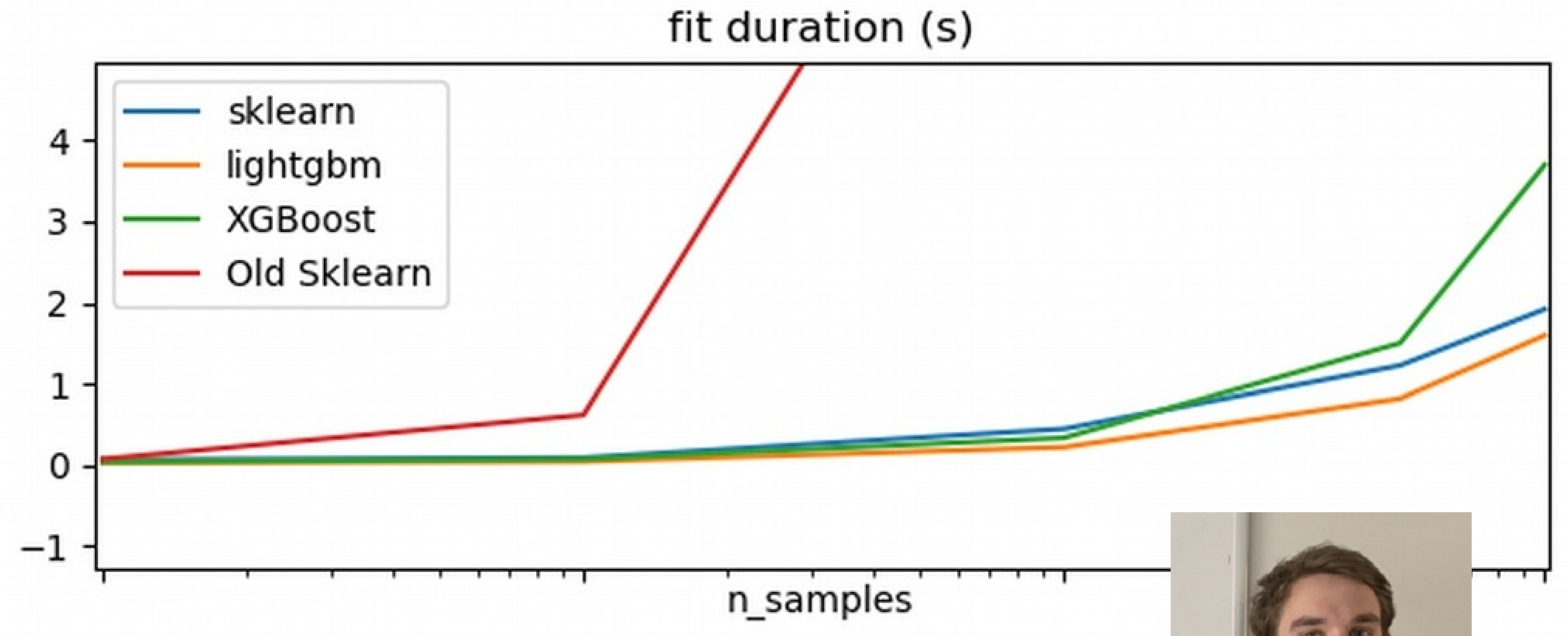
Automatic Model Search

Complex Models

- More Linear Models
- Random forest
- Gradient boosting
- Kernel methods



Side note: HistGradientBoosting



Successive Halving

- Given n configuration and budget B
- pick η=2 or η=3 (wording follows 2)
- Each iteration, keep best halve of configurations

<u>SuccessiveHalving</u> (Finite horizon)

input: Budget B, and n arms where $\ell_{i,k}$ denotes the kth loss from the ith arm, maximum size R, $\eta \geq 2$ ($\eta = 3$ by default).

Initialize: $S_0 = [n]$, $s = \min\{t \in \mathbb{N} : nR(t+1)\eta^{-t} \leq B, t \leq \log_\eta(\min\{R, n\})\}$.

For $k = 0, 1, \ldots, s$

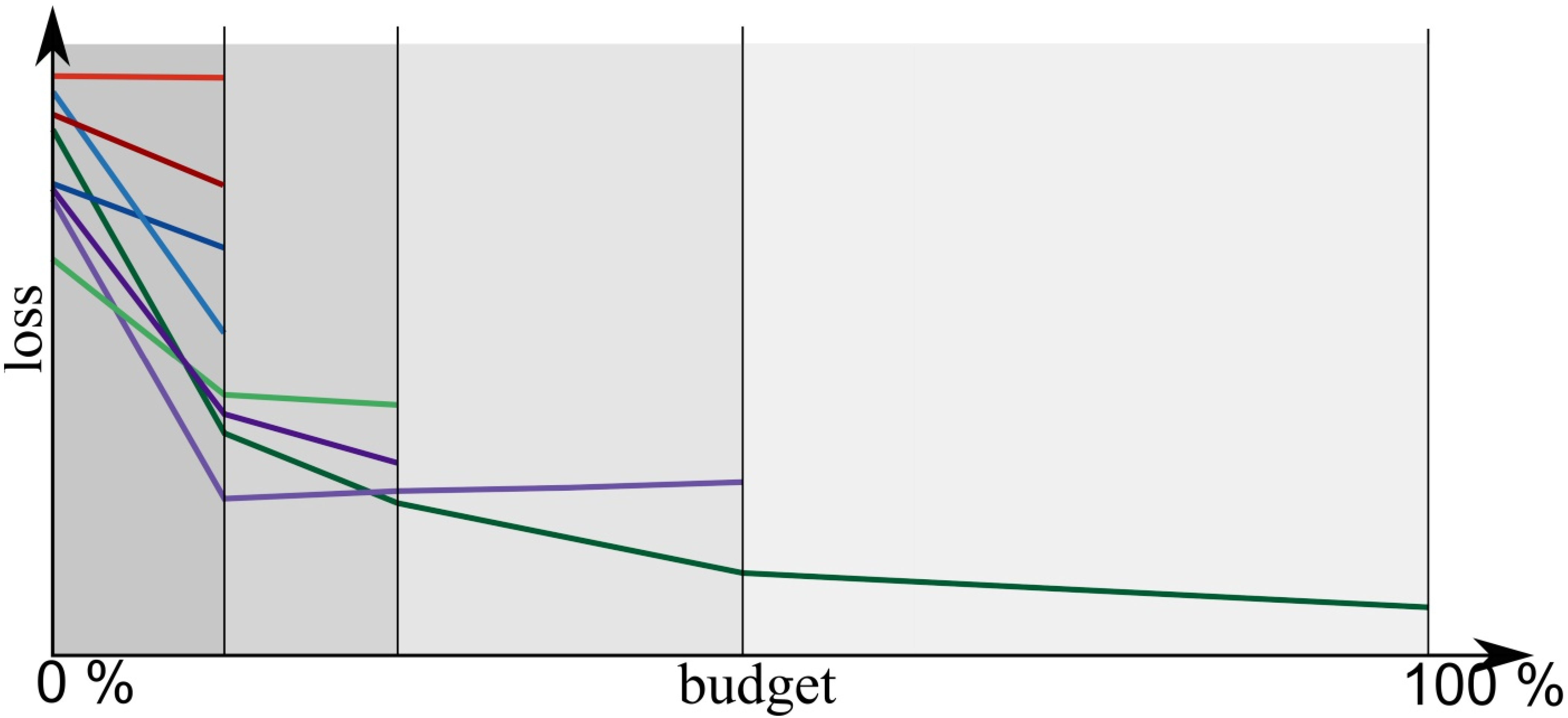
Set $n_k = \lfloor n\eta^{-k} \rfloor$, $r_k = \lfloor R\eta^{k-s} \rfloor$

Pull each arm in S_k for r_k times.

Keep the best $\lfloor n\eta^{-(k+1)} \rfloor$ arms in terms of the r_kth observed loss as S_{k+1}.

Output : $\hat{\imath}, \ell_{\hat{\imath},R}$ where $\hat{\imath} = \arg\min_{i \in S_{s+1}} \ell_{i,R}$

Successive Halving Illustrated



Portfolio creation

- Run Hyper-parameter optimization across models on large benchmark suite (OpenML-CC18)
- Evaluate all final models across all datasets
- Greedily create portfolio of best-performing, diverse models
- “Practical Automated Machine Learning
- for the AutoML Challenge 2018” Feurer et. al.

Model Explanation

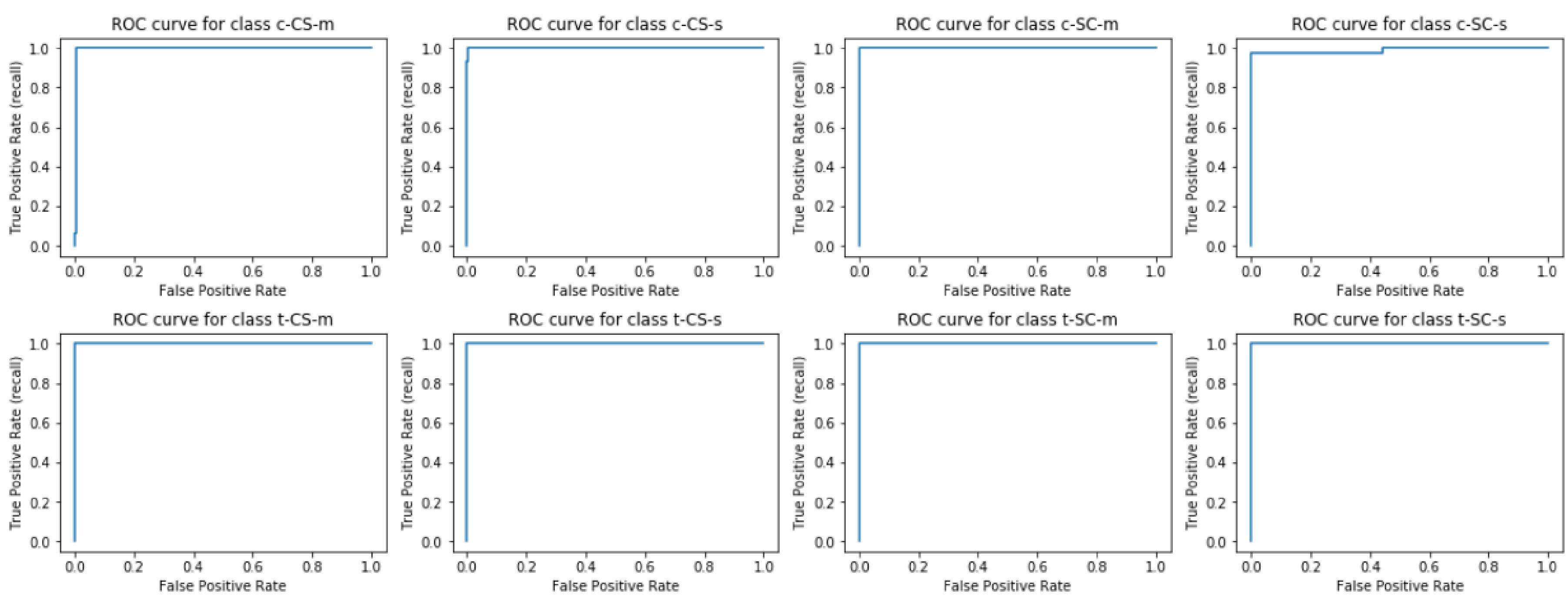
```python
from sklearn.model_selection import train_test_split
df_train, df_test = train_test_split(data)
ac = AnyClassifier().fit(df_train, target_col='target')
```

```python
import dabl
dabl.explain(ac, X_val=df_test, target_col='target')
```

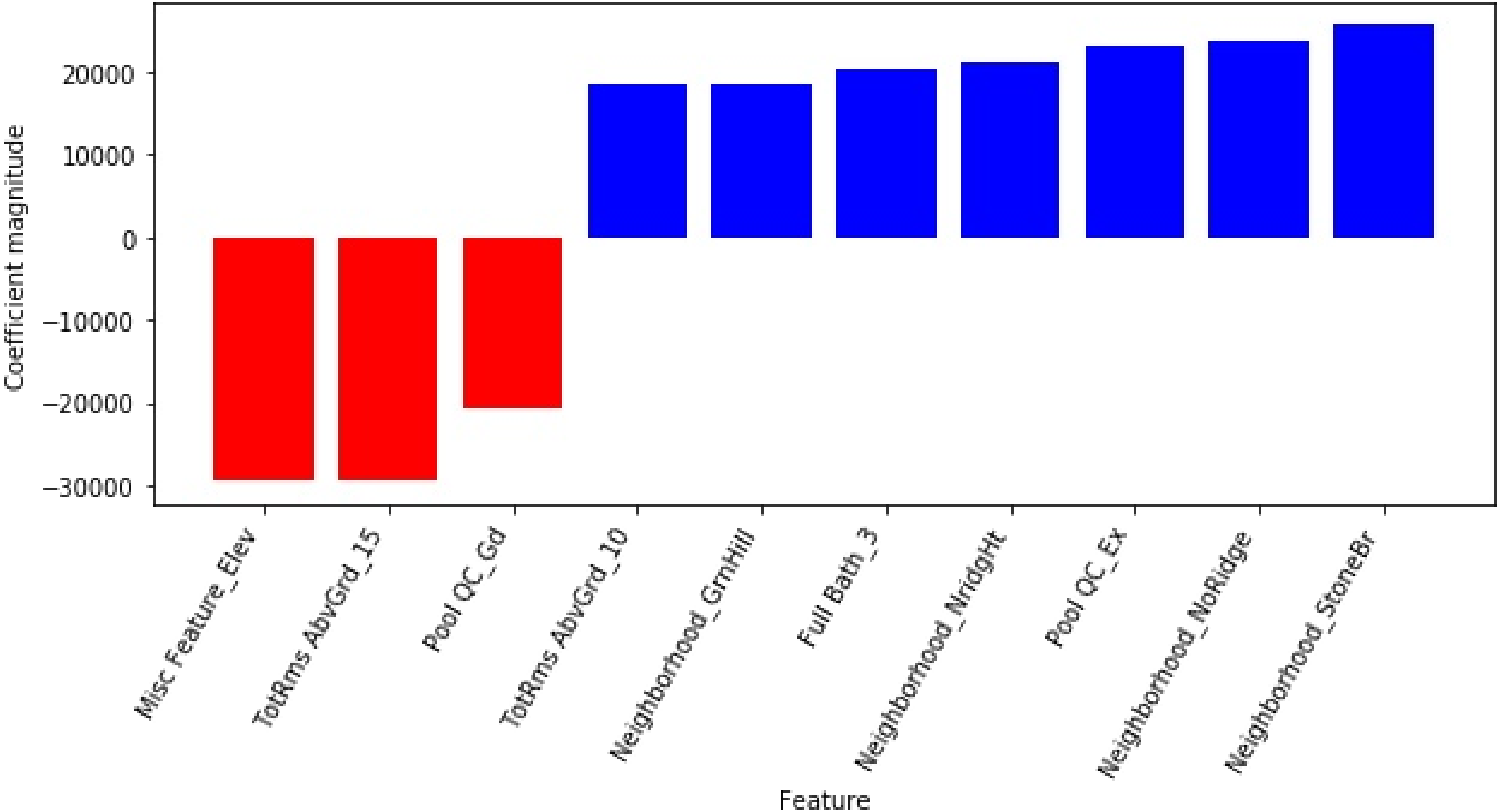
Metrics

	precision	recall	f1-score	support
c-CS-m	0.97	0.97	0.97	32
c-CS-s	0.94	1.00	0.97	31
c-SC-m	1.00	1.00	1.00	37
c-SC-s	1.00	0.94	0.97	34
t-CS-m	1.00	0.98	0.99	41
t-CS-s	1.00	1.00	1.00	21
t-SC-m	1.00	1.00	1.00	33
t-SC-s	0.98	1.00	0.99	41
accuracy			0.99	270
macro avg	0.99	0.99	0.99	270
weighted avg	0.99	0.99	0.99	270

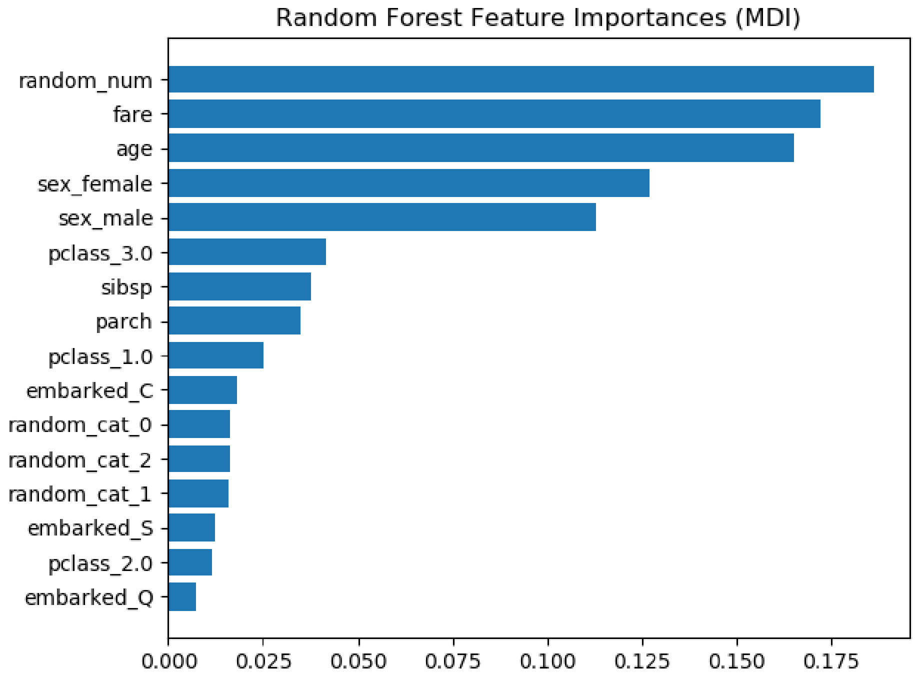
```
[[31  1  0  0  0  0  0  0]
 [ 0 31  0  0  0  0  0  0]
 [ 0  0 37  0  0  0  0  0]
 [ 1  0  0 32  0  0  0  1]
 [ 0  1  0  0 40  0  0  0]
 [ 0  0  0  0  0 21  0  0]
 [ 0  0  0  0  0  0 33  0]
 [ 0  0  0  0  0  0  0 41]]
```

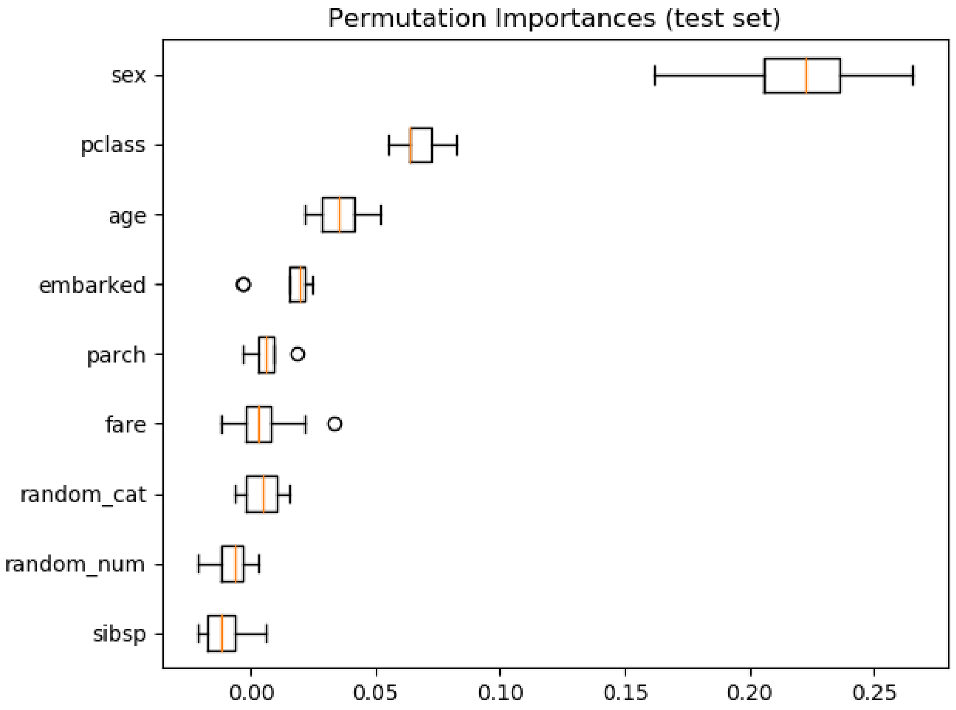


Coefficients / Feature importances



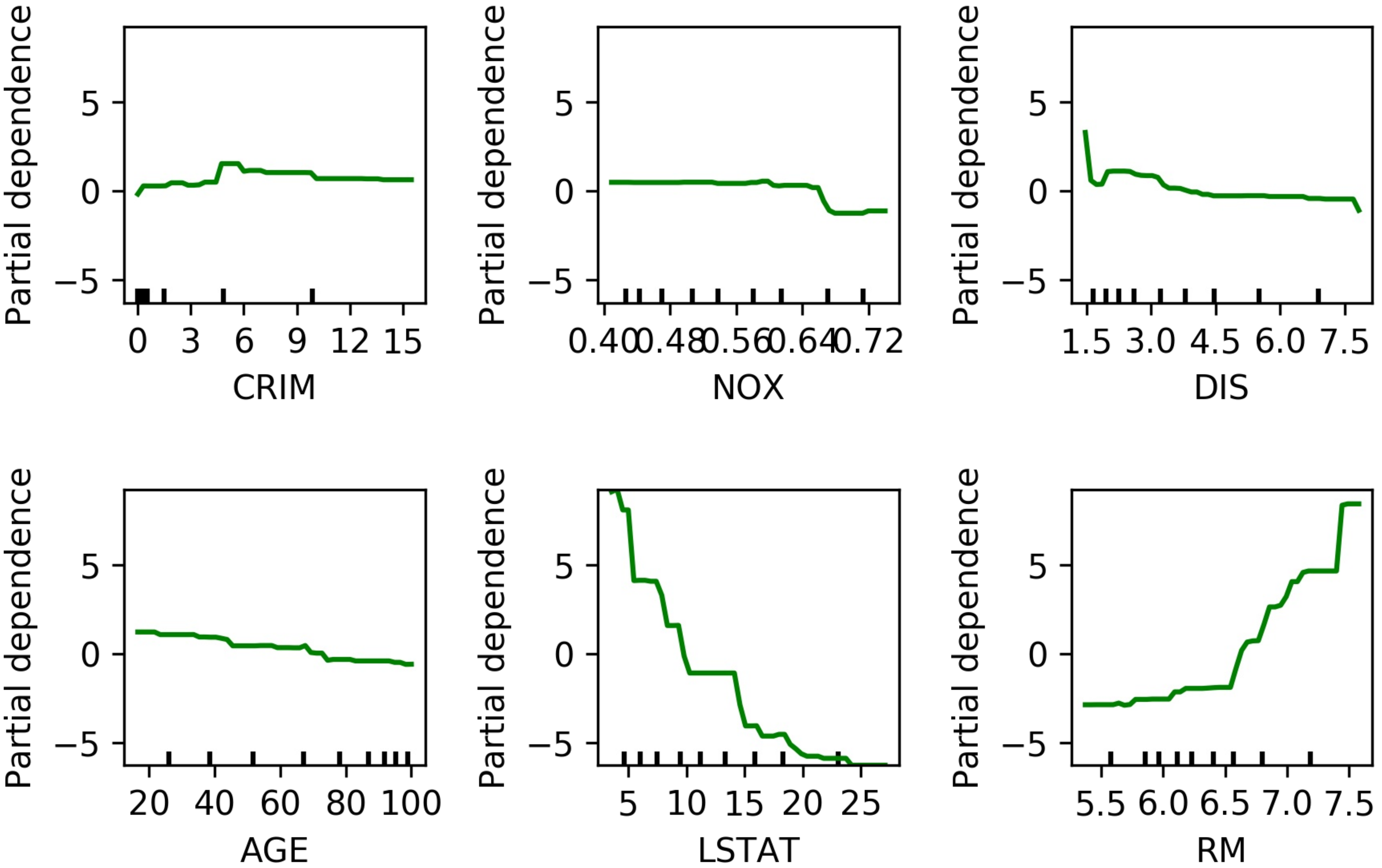
Permutation Importance





https://scikit-learn.org/dev/auto_examples/inspection/plot_permutation_importance.html

Partial Dependence Plots

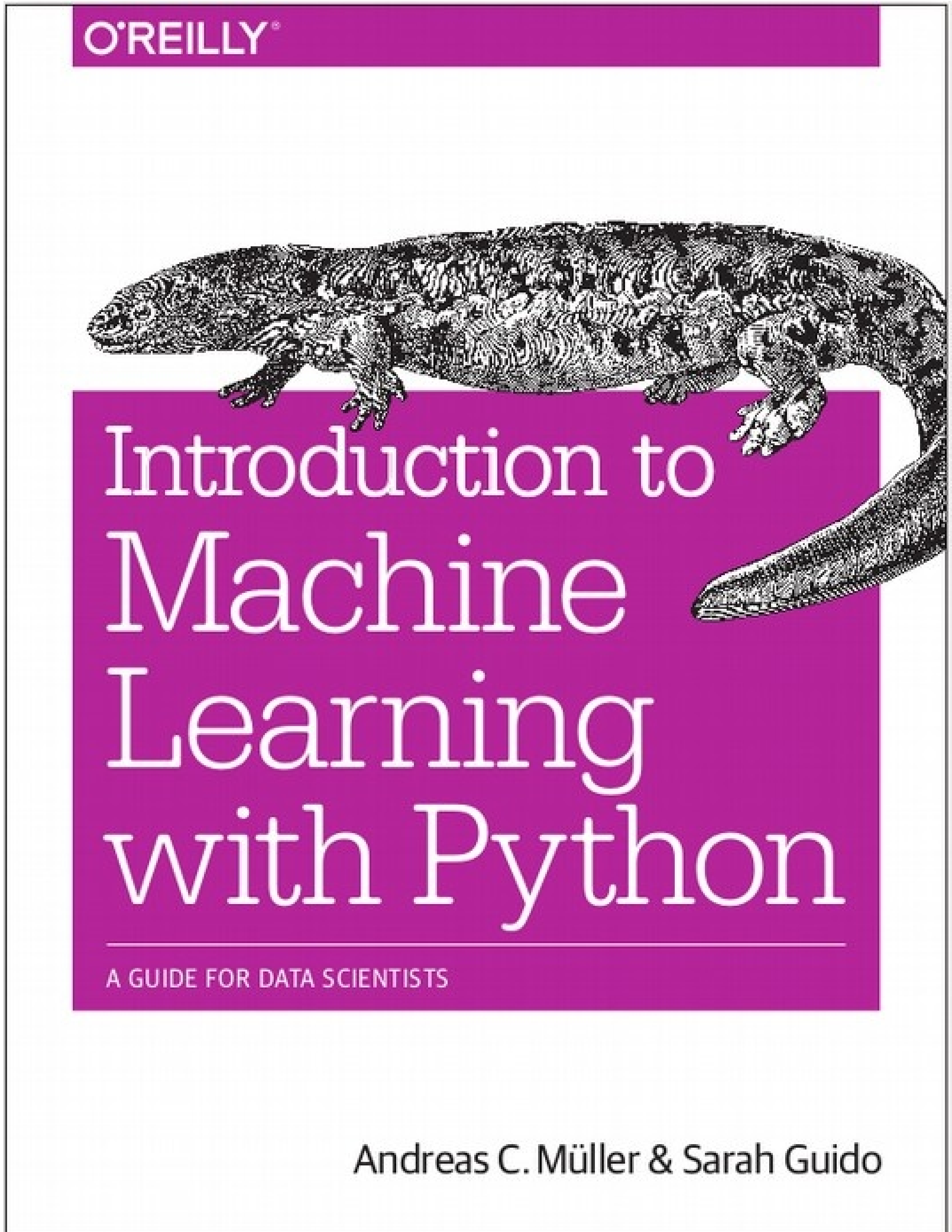


Future Goals

- Time sensitive portfolios

- Model compression
  / building explainable models

- Better model inspection



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